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Mathematical simulation of capacitive coupled radio-frequency discharge when high and low the pressure in the argon

Synopsis of dissertation

01.02.05 - Mechanics of fluid, gas and plasma

05.13.18 - Mathematical simulation, numerical methods and complexes of programs

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Relevance of the work. The low-temperature plasma is widely used to create micro- and nanostructures, as well as modification of surfaces. The advantage of plasma methods for material processing is a wide range of impact parameters. Different materials require different types of treatment, respectively, and the various conditions for maintaining the discharge. Some materials (e.g., carbonaceous and low-alloyed steels, polymers) can not with stand high temperatures, so one need to apply the so-called "cold plasma", at gas temperatures below 500 K. One of effective way for creating "cold plasma" is radio frequency capacitive (RFC) discharge at low pressure. The experimental results showed that RFC-discharge is effectively used to modify the natural polymeric materials such as leather, fabric. Creation of new facilities for the treatment of materials connected with the conduct of a large number of experimental studies on the selection of the parameters of plasma systems. Plasma characteristics can be obtained using experimental and computational experimentation. In this regard, great attention is paid to the development of mathematical models.

Objective of work: The aim is the creation of mathematical models of low-temperature plasma capacitive coupled radio-frequency discharge (CCRFD) in argon in a wide range of pressures. In this paper, generated numerical algorithms that are implemented in the form of software applications, the calculation of internal parameters of the discharge are produced.

The main provisions of work:

1. The self-consistent model of nonequilibrium capacitive coupled radio-frequency discharge low-temperature plasma in argon at high and low pressures are constructed, which include a variety of kinetic schemes of calculations adapted for low and high pressure.
2. Numerical algorithms for the implementation of the developed models based on the finite-dimensional approximation using schemes followed by application of iterative processes.
3. The set of programs for the task based on the proposed algorithms.

4. Numerical simulation results which have shown that the temperature change of the gas between the electrodes, greatly influences the ratio of the contributions of various plasma processes.

Scientific novelty.

1. Mathematical models in a wide range of capacitive coupled radio-frequency discharge pressure in the argon, which take into account the spatial variation of the gas temperature. Mathematical model includes equations for calculating the concentration of molecular ions and dimers in the case of high-pressure.
2. A numerical method is built. It is based on the use of implicit difference schemes, and an iterative process.
3. A software package that allows you to calculate the characteristics of the capacitive coupled radio-frequency discharge over a wide pressure range.
4. The conditions under which the mathematical model must take into account the heating of the gas.

Veracity. The reliability and validity of the results obtained in the thesis is based on an analysis of the physical model and the correct application of numerical methods. Numerical solutions are in good agreement with the known data from experiments those of other authors.

Theoretical and practical significance. The practical value lies in the possibility of using the developed application software for the calculation of basic parameters discharge at high and low pressures in order to manage the production process.

Theoretical value lies in the possibility of using the developed mathematical models and numerical algorithms for the analysis of processes, mechanisms in argon plasma over a wide pressure range.

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Approbation of the work.

The results were presented at professional conferences: FDM'14: Sixth Conference on Finite Difference Methods: Theory and Applications (Lozenetz, 2014 г.); Proceedings of the IX international conference on nonequilibrium processes in nozzles and jets (Alushta, 2012); X INTERNATIONAL CONFERENCE "Mesh Methods for Boundary-Value Problems and Applications" (Kazan,2014); INTERNATIONAL CONFERENCE "Advanced mathematics, Computations and applications-2014"(Novosibirsk,2014);international Zvenigorod Conference on Plasma Physics and Controlled Fusion (Zvenigorod, 2013-2015): the 14th Israel Conference on Plasma Science abd Applications (iarael,2012); INTERNATIONAL CONFERENCE ICPTSMODM (Kazan, 2012); et al.

The structure and scope of work. Thesis is presented on 123 pages, consists of introduction, three chapters, divided into paragraphs, conclusions, a single application and a list of literature includes 165 works.

Content of work.

Relevance, purpose, scientific novelty specified in the introduction, the main provisions are presented, a summary of the chapters is given **in the introduction.**

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The **first chapter** provides an overview of works devoted CCRF-discharge. Results of experimental and theoretical studies CCRF-discharges, their characteristics in different gas atmospheres with different materials of the electrodes and the distances between them, different pressure ranges given in this chapter Considerable attention is paid to the description of known mathematical models CCRF-discharge, and glow discharge. Details considered plasma-chemical reactions that are necessary for simulation of argon plasma.

review of work on the mathematical modeling of phenomena in electric discharges is given in the work. Review of work on the mathematical modeling of phenomena in electric discharges is given in this chapter. Analysis of the literature showed that, despite the large number of published works, many questions CCRF-discharge, simulation is still poorly understood. For example, simulation RF- discharge in a wide range of pressures, for analyze the physical and chemical processes in them. Creation of software packages for the simulation of radio-frequency discharge in a wide pressure range for use in dealing with a variety of applications.

Self-consistent mathematical model CCRF-discharge built in the nonlocal approximation at reduced pressures in argon in the **second chapter**. The model presented here describes a capacitive coupled RF discharge between two plane-parallel electrodes, one of which is grounded and the other connected to RF-generator, the distance between the electrodes is less than the size of the electrodes themselves. In these conditions the electric field close to the potential and the discharge is uniform along the electrode that allows you to apply a one-dimensional model. Estimates time of dissipation of energy of the electrons and the relaxation length of the electron energy at lower pressures indicate that the need to use non-local approach for modeling RF discharge. The model includes the balance equation for the electron gas metastable atoms, atomic ions, the Poisson equation for the potential of the electric field, the balance equation for the electron energy, as well as stationary heat equation atomic ion gas for averaged parameters. The coefficients of velocity processes under electron impact calculated using BOLSIG + program taking into account the electron-electron collisions, depending on the electron temperature and the degree of ionization.

The following properties CCRF-discharge interfere with the development of numerical methods for solving the problem:

1. systems consist of different types of problems;

2. different time frames for change characteristics CCRF-discharge of low pressure interfere with the development of numerical methods.
3. large gradients of solutions of equations and dependent coefficients
4. The proposed system is a non-linear problems both for individual equations within it, and as a whole.
5. Required to carry out the calculation of flows in regions strongly varying coefficients, in the presence of large gradients of solutions.

Review of the numerical methods to overcome these problems is given in this chapter.

The computational algorithm for solving a nonlinear system was built. The approximate method was used for solving of the nonlinear problem which is based on the finite-dimensional approximation of the problem with the help of difference schemes with subsequent application of the iterative process for its implementation. For initial value problems the implicit finite-differenc scheme with equal ideally meshes partition was used. The operator of convective transport was approximated by methods directional differences with the multi-directional movement of ions and electrons. Application of integral-interpolation method for constructing finite-difference scheme provided its conservative. The resulting non-linear finite-difference scheme was solved by the method of Seidel-type. Nonlinearity of the electron temperature in the coefficients was moved to the lower layer. In addition, linearization quadratic terms in the balance equations of meta-stable atoms was carried out. Density streams for ion and electron gas is calculated by the method such as Gummel.

The software package that implements the numerical algorithm for finding the parameters of non-stationary low-pressure radio-frequency discharge in the one-dimensional approximation was built. Matlab environment was used to create a software package. The results of calculations performed using the developed software package was implementation, and comparative analysis with the data of other authors was held. The results of calculations CCRF-

discharge in the plasma torch with an interelectrode distance of 0.022 meters, at a pressure of 13.3 Pa, the amplitude of the applied voltage is 65 V and the results of the calculations at a pressure of 133 Pa, the amplitude of the applied voltage is 100 V, the inter-electrode distance of 0.0254 m are presented in this chapter.

In the **third chapter**, the model CCRF-discharge in the local approximation at high pressures was built. plasma chemical reactions involving dimers and molecular ions in model CCRF-discharge at elevated pressures in argon was justified. Contained in chapter self-consistent model CCRF-discharge at elevated pressure includes a balance equation for the electron gas metastable atoms, molecular and atomic ions, the kinetic equation for the dimer argon and neutral atoms, the Poisson equation for the electric field potential, as well as stationary heat equation atomic-ion gas with the boundary conditions of heat transfer calculated by the average parameters. The coefficients of velocity processes under electron impact depends on the local value of the reduced electric field and the degree of ionization with electron-electron collisions. numerical algorithm solutions of the mathematical model based on the finite-dimensional approximation of the problem with the help of difference schemes with a subsequent application for its implementation of the iterative process was offered. And difference schemes for the initial, boundary and initial-boundary problems of the non-linear system describing the considered model CCRF-discharge were given. Numerical results at atmospheric pressure, and the interelectrode distance of 2 mm were made. Comparative analysis of these results with other known data was given. In addition, the results of calculations during the inter-electrode distance of 2 cm and the analysis of these results was given.

In **conclusion,** we present the main results of:

1. Numerical calculations showed that the change in the temperature of the gas in the electrode space begins to significantly affect the plasma-chemical processes.
2. self-consistent mathematical model CCRF-discharge in nonlocal approximation under reduced pressure argon was built. processes involving electrons are taken depending on the electron temperature and the degree of ionization, electron-electron collisions.
3. self-consistent mathematical model CCRF-discharge in the local approximation at elevated pressures in argon built. Coefficients for electrons are taken depending on the values a local field and the degree of ionization. spatial variation of the gas temperature is taken into account in the mathematical model. The presence of molecular ions and dimers is taken into account in the model
4. Numerical algorithms for solving mathematical models developed.
5. software package for the calculation of CCRF-discharge parameters was developed
6. qualitative and quantitative comparison of the numerical calculations are carried out with the known data. comparison confirms the performance and reliability of the developed complex programs. Applications can be used for analyzing the physico-chemical processes in CCRF-discharge in a wide range of pressures.

Publications.

Materials of the thesis were published in 30 papers.